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Theoretical Solid State Physics and Statistical Mechanics Group I

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Research Activities

(I) ELECTRONIC STRUCTURES OF SEMICONDUCTORS, SEMIMETALS AND METALS

a. Black Phosphorus (C. Kaneta, H. Asahina, T. Sasaki, H. Katayama-Yoshida, K. Shindo and A. Morita)[1),2)]

(i) We have successfully explained the optical properties of black phosphorus such as UPS, XPS, optical reflectivity in visible and VUV regions using the results of the self-consistent-pseudopotential band calculation. (To appear in J. Phys. C17 (1984)). We have also calculated the polarized soft X-ray K emission and absorption spectra of black phosphorus using experimental spectra obtained by Sagawa group recently. (To appear in Phys. Rev. B29 (1984)).

(ii) We have calculated the anisotropic electrical conductivity of black phosphorus using the deformation potential model and a realistic phonon model (see (iv)) and have discussed from the band theoretical point of view the origin of large anisotropy in the deformation potential constants needed to explain the anistropic electrical conductivity.

(iii) The electronic properties and phase changes of black phosphorus under pressure have been studied in terms of the self-consistent-pseudopotential band calculation. (To appear in Proc. Inter. Symp. on Solid State Phys. under Pressure).

(iv) So far we have calculated the lattice dynamics in black phosphorus. Now we are calculating it using the bond charge model in order o treat infrared active optical phonon modes more reasonably.

b. Electronic Structure of Deep Impurity States in Semiconductors (H. Katayama-Yoshida and K. Shindo)

(i) The spin-polarized calculation of the electronic structure around a positive muon and boron at the tetrahedral interstitial site in silicon is carried out using the local spin-density functional formalism and LCAO-Green's function method. Bonding hyper-deep impurity states below the valence band and antibonding deep ones in the band gap caused by the sp-hybridization contribute to the reduction of the hyperfine coupling constant, A. The calculated value of A is in good agreement with the μSR experimental data.[3)-6)]

(ii) Electronic structure around a chromium at the substitutional garium site in garium arsenide is calculated by means of the same method as (i) in the case of non-magnetic states. We find the bound states in the first and second gaps caused by the strong pd-hybridization.

c. Electronic Structure of Graphite Intercalation Compounds (H. Mitani and A. Morita)

In order to explain the de Haas-van Alphen effect in alkali-metal graphite intercalation compounds, we are trying to extend Shimamura and Morita's model so as to take account of interactions between carbon layers separated by an intercalant layer. We have shown that the hopping between carbon layers sandwiching an intercalant layer is important.

d. Effect of Impurities on Superconductors (Y. Okabe)

(i) The Shiba-Rusinov theory of magnetic impurities in a superconductor is investigated, with special attention paid to the role of potential scattering term.[7)] The effect of magnetic impurities on superconductors with energy-gap anisotropy is studied using the Shiba-Rusinov theory. The transition temperature T_c and the jump in specific heat at T_c are calculated.[8)]

(ii) Using the Anderson model in the nonmagnetic limit, we have studied some properties of the superconducting virtual-bound-state alloys.

The calculated properties are the transition temperature T_c, the jump in specific heat at T_c, the electronic density of states, and the tunneling conductance. Special attention is paid to the systematic variation of these properties with the resonance width.[9),10)]

(iii) The effect of nonmagnetic impurities on antiferromagnetic superconductors has been investigated in detail. We show the apperance of bound states due to impurities and the growth of the "impurity band" with the increase in impurity concentration. The "dirty"-limit behavior of the system and the condition for the apperance of the gaplessness are discussed analytically.[11)]

(II) CRITICAL PHENOMENA

a. Effect of Surfaces on Critical Phenomena (K. Ohno and Y. Okabe)

The critical behavior of the classical n-vector model on the semi-infinite lattice has been studied with the 1/n expansion scheme. Generalizing the 1/n expansion method developed by Abe to the semi-infinite system, we calculate several surface critical exponents for the ordinary and special transitions.[12)-14)] Some scaling relations proposed by Bray and Moore were shown to be violated at O(1/n). We also discussed the critical behavior of the surface susceptibilities by means of the high-temperature expansion.[15)]

b. Monte Carlo Study of Critical Phenomena (M. Kikuchi and Y. Okabe)

We performed the Monte Carlo simulation of the three-dimensional Ising model with free surface. The critical behavior of layer magnetization, layer susceptibility and local susceptibility near the ordinary transition point was investigated. The universal property of the surface critical exponents and the critical amplitude ratios were confirmed.

(III) ELECTRONIC STRUCTURES AND TRANSPORT PORPERTIES OF LIQUID METALS, LIQUID ALLOYS AND OTHER DISORDERED SYSTEMS

a. Electronic Structure of Liquid Heavy Polyvalent Metals (A. Nishikawa and K. Niizeki)

We have calculated the electronic structure of liquid thallium

from first principles, as a first step of a series of investigations of the electronic properties of the heavy polyvalent metals (Hg, Tl, Pb and Bi) in the liquid states. We have obtained the electronic densities of states and the dispersion curve by the relativistic version of the KKR-EMA.[16] Our results are compared with the recent photoemission data.

b. Electrical Conductivity of a Disordered System (K. Niizeki)

An expression for the velocity matrix of an electron in the tight-binding approximation is derived for a disordered system by taking the nonorthogonality between atomic orbitals into account. The velocity matrix has a complicated dependence on the atomic configuration. However, the velocity matrix can be shown to be replaced in the Kubo-Greenwood formula for the DC conductivity by an effective velocity matrix which has explicit energy dependence but has a simple configuration dependence.[17]

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2) Electronic properties of black phosphorus, A. Morita, Kotai Butsuri 19 (1984) 63 (in Japanese).
3) Hyperfine interaction of light interstitial impurity nuclei in silicon, H. Katayame-Yoshida and K. Shindo, Hyperfine Interactions 15/16 (1983) 539 (Proceedings of the 6th International Conference on Hyperfine Interactions, Groningen, 1983).
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5) Electronic structure of positive muon, H. Katayama-Yoshida and K. Shindo, Hyperfine Interactions 17-19 (1984) 581 (Proceedings of Yamada Conference on μSR, Shimoda, 1983).
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9) Specific heat jump for superconducting virtual bound state alloys, Y. Okabe and A.D.S. Nagi, Solid State Commun. 46 (1983) 639.

10) Some properties of superconducting virtual-bound-state alloys, Y. Okabe and A.D.S. Nagi, Phys. Rev. B28 (1983) 2455.

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12) Surface critical exponents in 1/n expansion, K. Ohno and Y. Okabe, Phys. Lett. 95A (1983) 41.

13) The 1/n expansion for the special transition in semi-infinite systems, K. Ohno and Y. Okabe, Phys. Lett. 99A (1983) 54.

14) The 1/n expansion for the n-vector model in the semi-infinite space, K. Ohno and Y. Okabe, Prog. Theor. Phys. 70 (1983) 1226.

15) High-temperature expansion of surface critical exponents for classical n-vector model, K. Ohno and Y. Okabe, Phys. Lett. 95A (1983) 38.

16) The relativistic KKR-EMA densities of states of liquid heavy polyvalent metals, A. Nishikawa and K. Niizeki, J. Non-Cryst. Solids 61/62 (1984) 1331.

17) A general expression for the DC conductivity of a disordered system in the tight-binding approximation : a treatment of the non-orthogonality between atomic orbitals, K. Niizeki, M. Itoh and M. Watabe, J. Phys. C16 (1983) 5829.

Doctor Thesis (March 1984)

D1) Theoretical studies on the critical phenomena at surfaces, Kaoru Ohno.

Master Thesis (March 1984)

M1) Pressure effects on the electronic structure of black phosphorus, Taizo Sasaki